

Molecular Dynamics Simulations of Ion Sputtering of Metal Surfaces

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Introduction

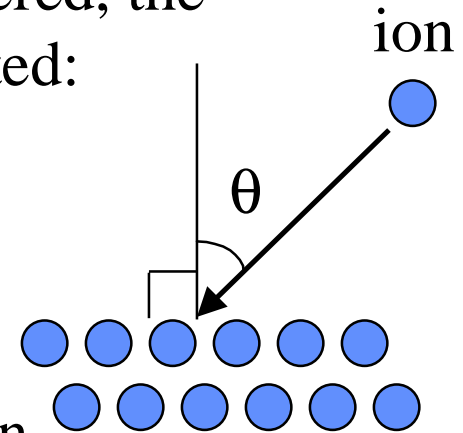
- Ionized physical vapor deposition (PVD) is used in Cu interconnect technology in the manufacture of integrated circuits.
- The interaction of energetic ions with the growing Cu film is not well characterized by a constant sticking coefficient or sputter yield (one that is independent of ion impact angle or energy).
- More detailed information is necessary as input for realistic feature scale modeling of film coverage in the metallization of micron-sized features (vias and trenches) in integrated circuits.

Summary of Molecular Dynamics Simulations

1. Conditions are representative of an ionized PVD process; Cu and Ar ions generated in the plasma are accelerated through a plasma sheath potential at the surface of the substrate.

2. For each impact angle θ and energy considered, the following averaged properties were calculated:

- sputter yield
- sticking probability
- thermal accommodation coefficient
- average reflection angle of the impact ion
- average emission angle of the sputter products



Details of the Molecular Dynamics Simulations

1. Interatomic potentials

- Embedded atom method (EAM) for Cu-Cu interactions
- Ziegler-Biersack-Littmark pair potential for Ar-Cu interactions
- Moliere pair potential for Ar-Ar interactions
- Neutral-atom potentials are appropriate; the incident ion is neutralized well before impact by a fast Auger process.

2. Simulation

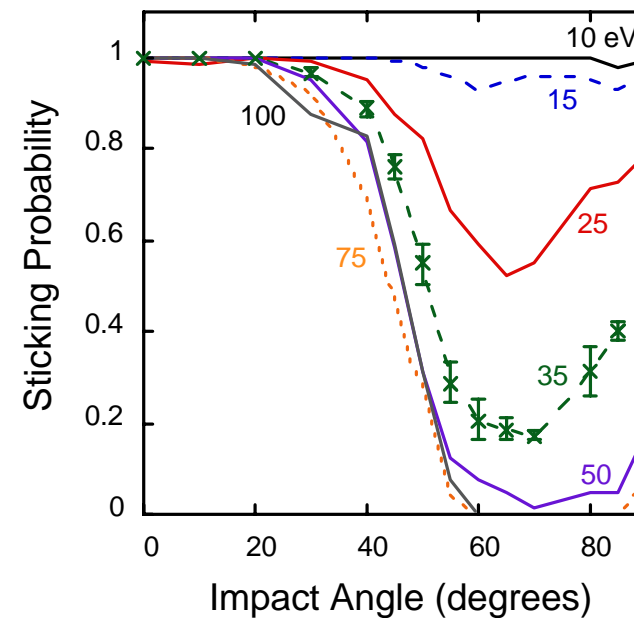
- 972 Cu atoms, fcc crystal, 12x9x9 atoms (x,y,z), 108 atoms per layer
- Periodic boundary conditions in x and y, free in z (normal to surface)
- Bottom two layers (216 atoms) rigidly fixed at all times
- An impact atom with desired incident energy and impact (polar) angle was positioned randomly in (x ,y) and azimuthal angle above the surface.
- For each impact angle and energy, a series of 150 impact events were run, using a pristine $T = 300$ K Cu (111) surface for each event.
- Results were insensitive to the size of the integration time step, the use of a larger substrate, or the use of a thermostat to dissipate deposited energy.

MD simulations predict sticking probability as a function of both energy and impact angle

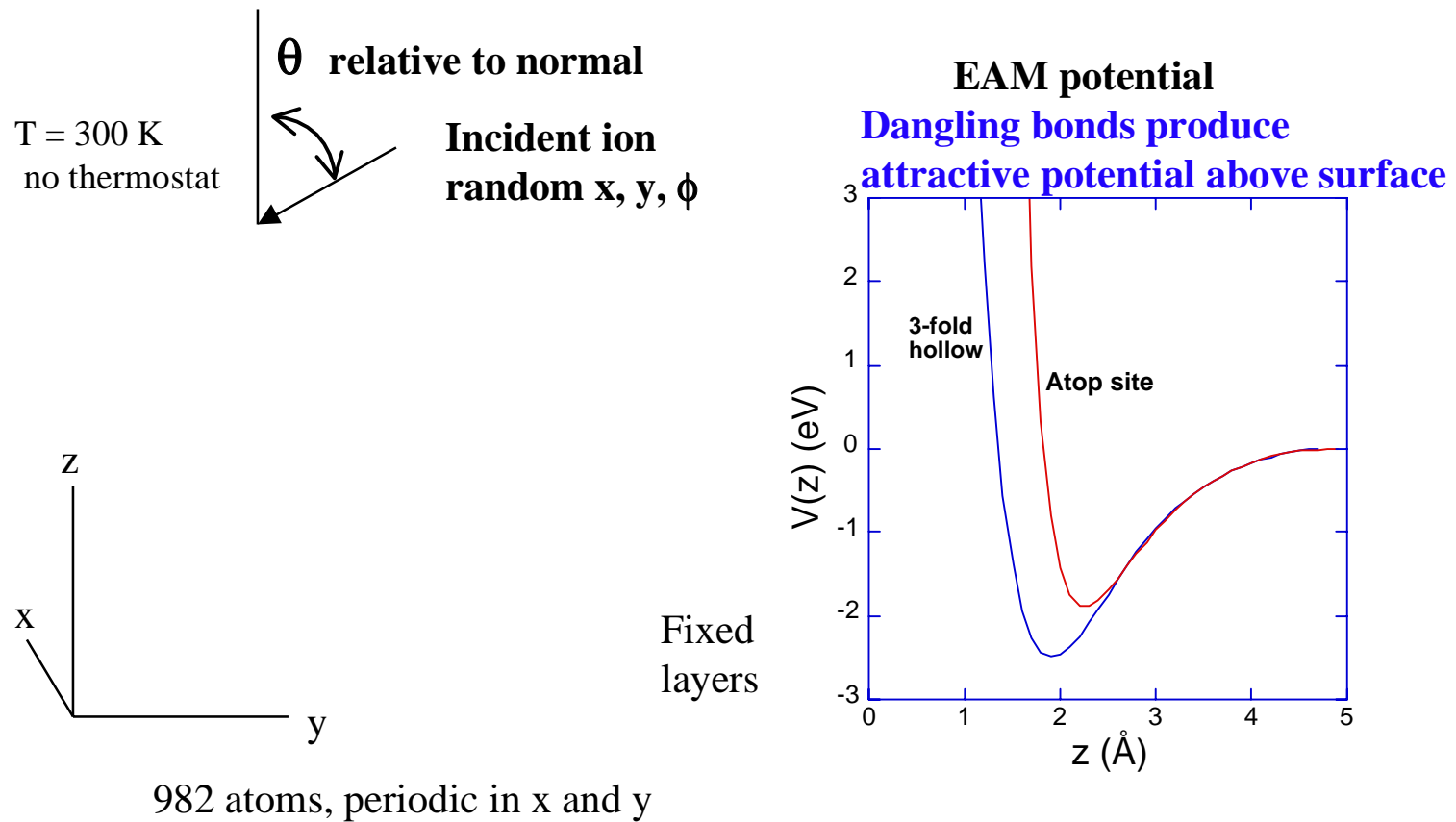
Within 20° of normal, everything sticks

Minimum in sticking probability at $\sim 70^\circ$

Sticking probability
increases for impact
angles $> 70^\circ$

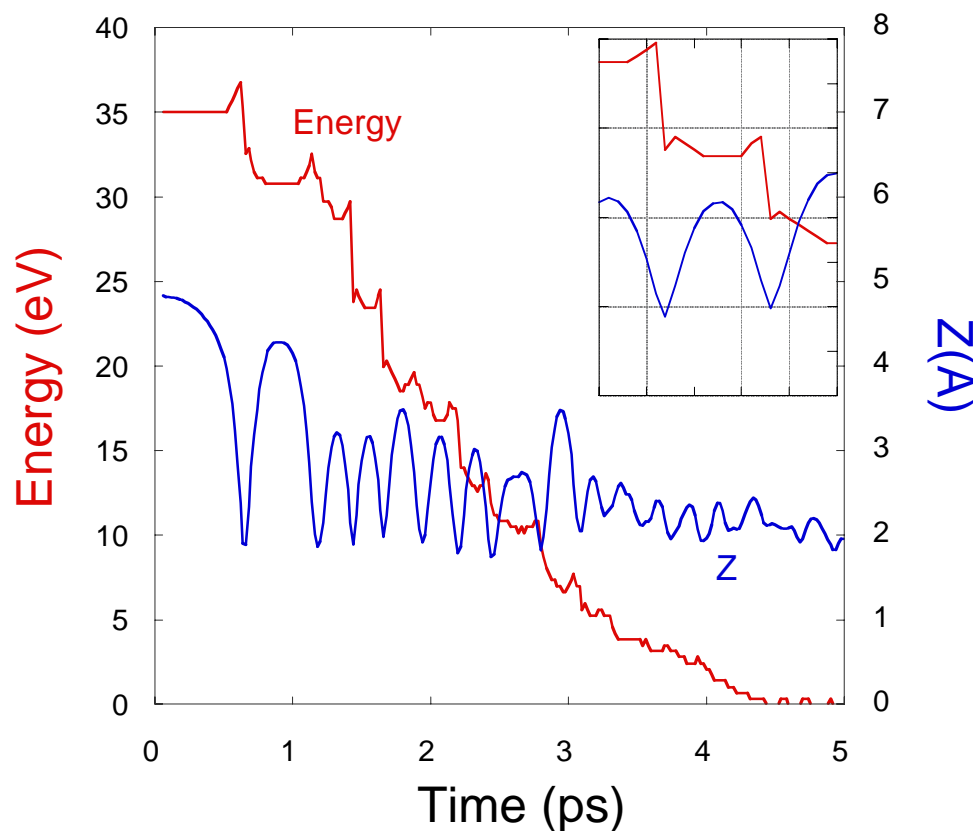


Surface trapping and desorption simulated with Molecular Dynamics



Surface Trapping: Energy loss correlates with oscillation

- 35 eV Cu atom incident on Cu(111), $\theta = 90^\circ$
- Atom oscillates 2 - 3 Å above surface, $\tau \sim 0.2$ ps
- Energy loss correlates with minimum of oscillation
- Average energy loss rate is constant to 10 eV



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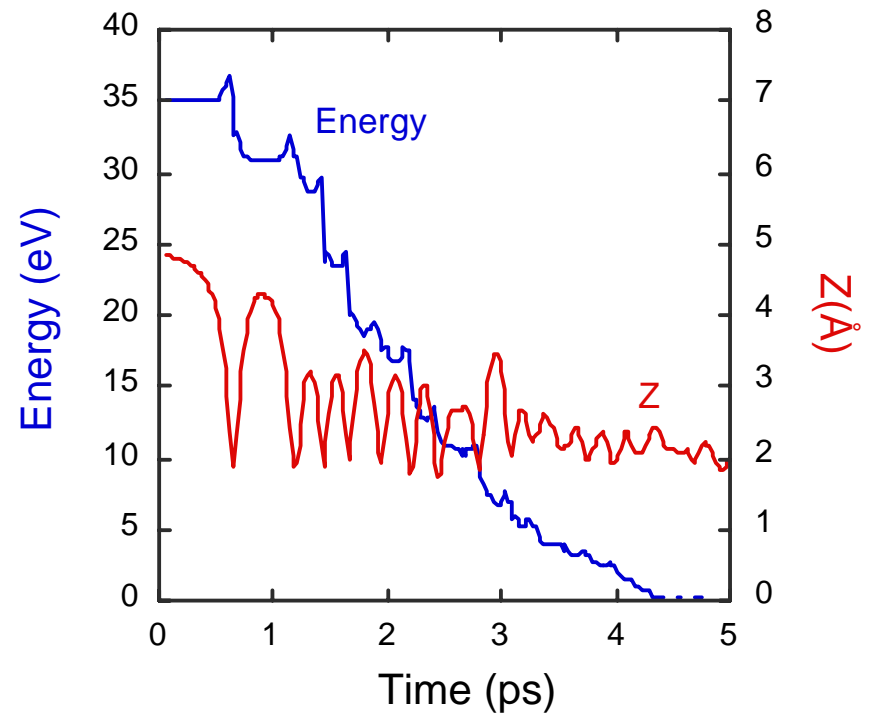
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Upturn in sticking coefficient is due to surface trapping

Impact atom can become trapped, oscillating
normal
to the surface

Average energy loss is piecewise linear

Atom can traverse hundreds
of Å before adsorbing



Phenomenological model developed to describe surface trapping

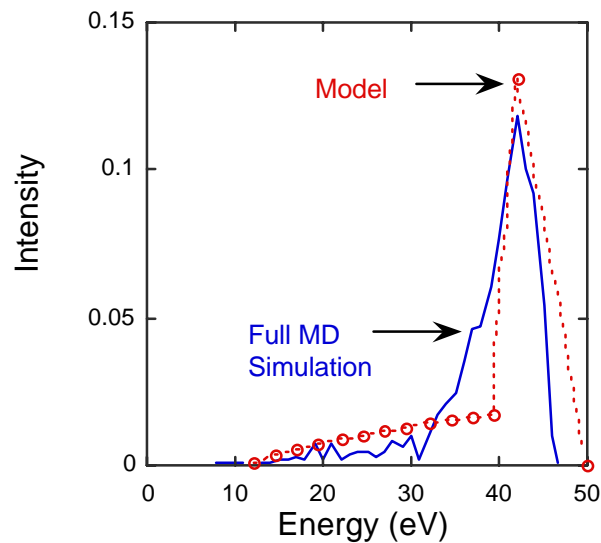
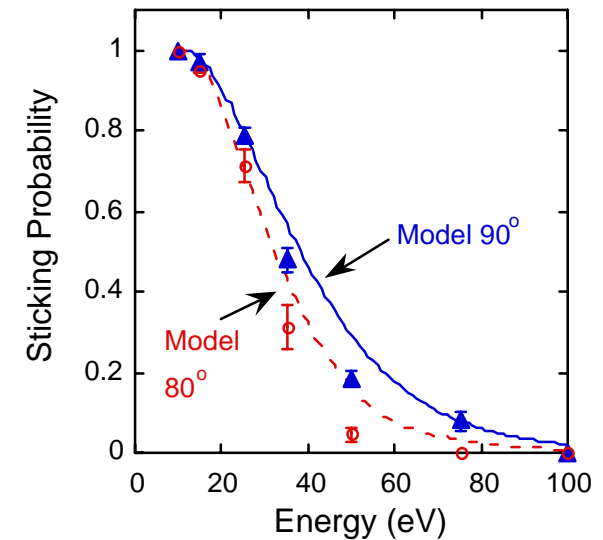
- MD simulations give energy loss and desorption probability for a single “bounce”
- Equations solved iteratively from impact energy down to 10 eV
- Energy loss is independent of energy after initial impact for Cu/Cu and the same for both (001) and (111) surfaces
- Desorption probability increases with energy

$$P_{stick} = \prod_{i=1}^n (1 - P_{desorb}(E_i))$$

$$E_i = E_o - i\Delta E$$

Predictions by phenomenological model agree with full MD results

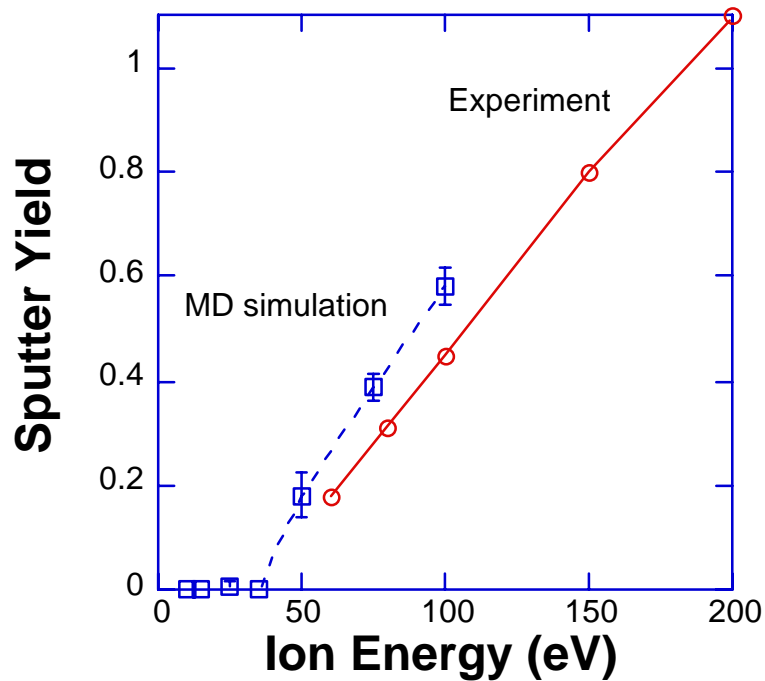
Comparison of model and full MD:
Sticking probability vs. energy for
 Cu^+ on $T = 300\text{K}$ Cu(111) at 80° and
 90° incidence



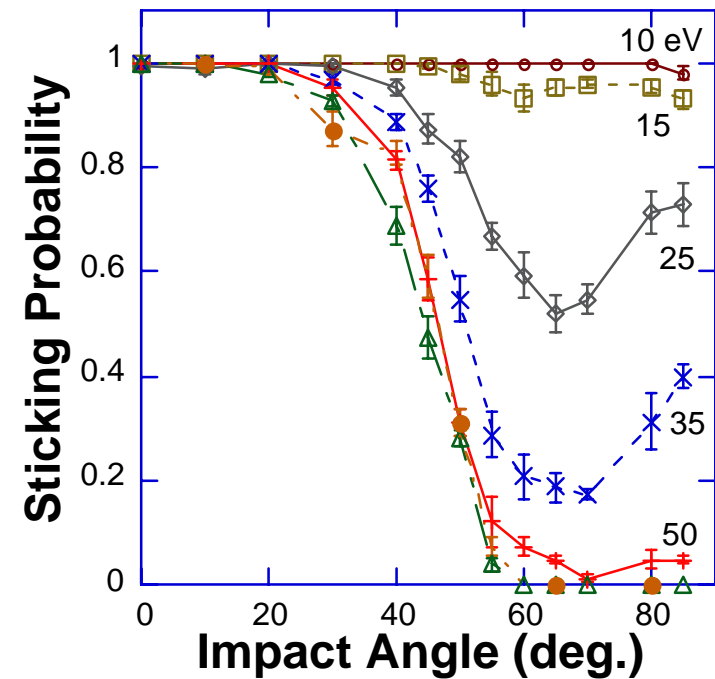
Comparison of model and full MD:
Predicted reflected energy
distribution for 50 eV Cu^+ on
Cu(111) at 80° incidence

Cu Ions Impinging on a Cu(111) Surface: Molecular Dynamics Simulations

Sputter Yield
(Normal Incidence)

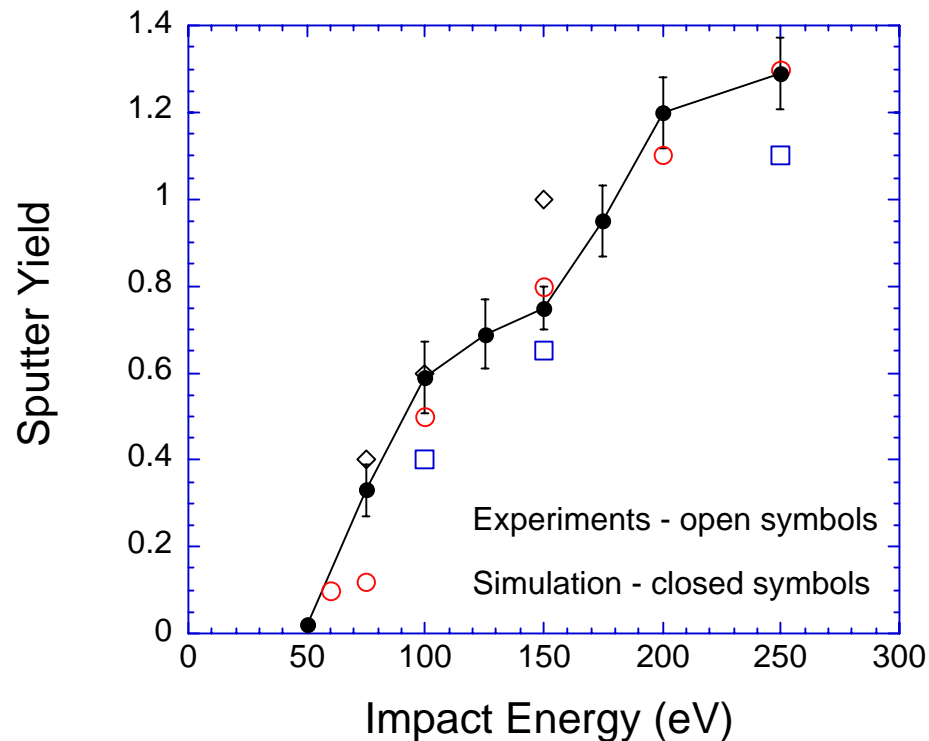


Sticking Probability
(Various Impact Energies)

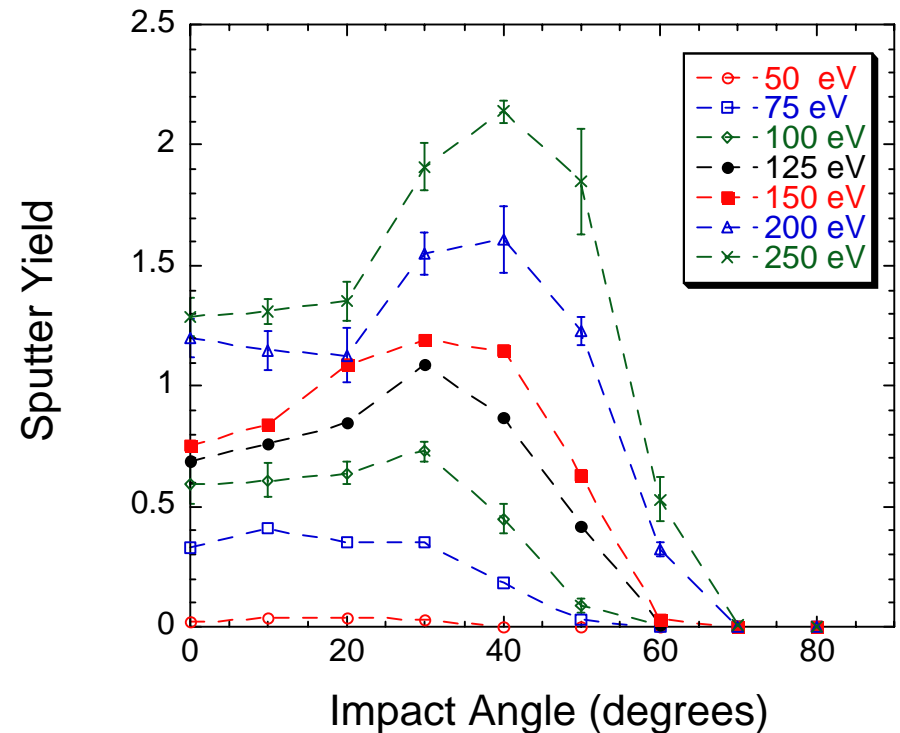


Ar Ion Sputtering of a Cu(111) Surface: Molecular Dynamics Simulations

Normal Incidence



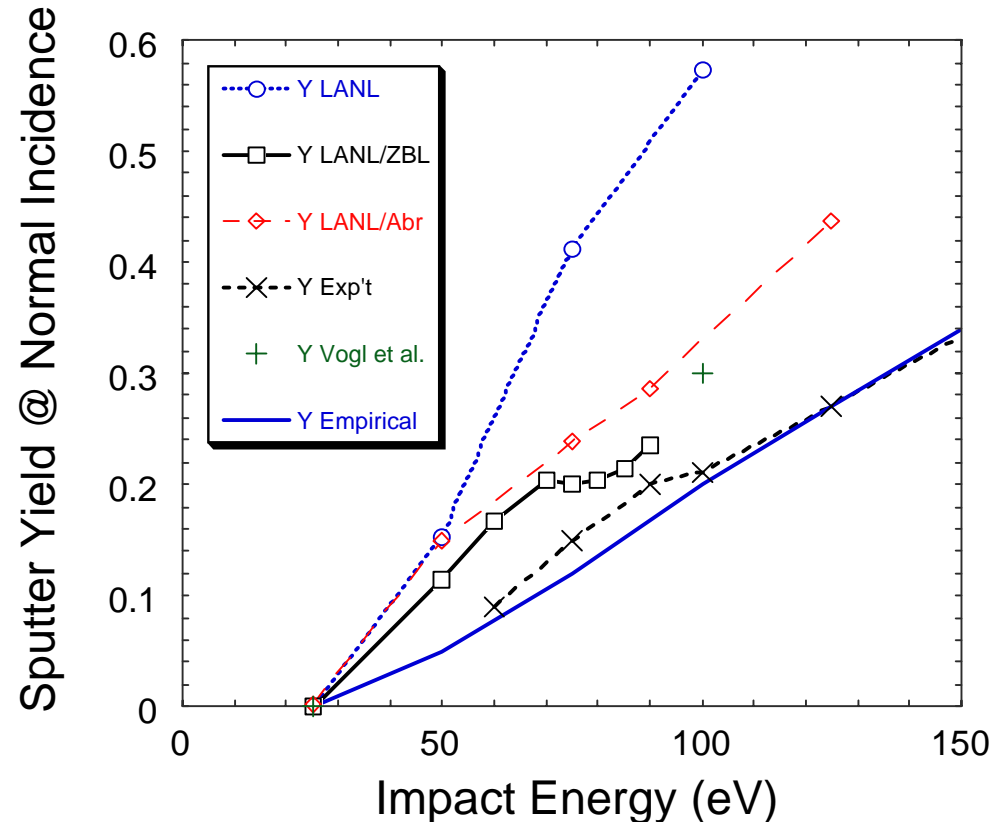
Various Impact Energies



Al Ion Sputtering of a Al(111) Surface

Key for figure:

- MD/Interatomic Potential:
LANL=LANL EAM
LANL/ZBL = EAM + ZBL Pair
LANL/Abr = EAM + Abrahamson Pair
Vogl et al. = Adams/Ercolessi EAM
+ Abrahamson Pair
- Experiment:
Empirical = “Universal” fit to data for
many ions/metals
Exp’t = data for Al+/Al



- For Al dimers: LANL/ZBL agrees well
with accurate electronic structure
density functional calculations

Conclusions:

Molecular Dynamics Simulations of Cu and Ar Ion Sputtering of Cu (111) Surfaces

- The following averaged properties were computed: sputter yield, sticking probability, thermal accommodation coefficient, reflection angle of the impact ion and emission angle of the sputter products.
- Sticking probabilities and sputter yields were found to vary as a function of both impact angle and energy.
- Calculated sputter yields at normal incidence for both Ar and Cu sputtering of Cu were in good agreement with experiment.
- For grazing incidence impacts, the sticking probability for energetic Cu ions ($E < 100$ eV) decreases then increases as a function of impact angle. Similar behavior has been observed in the trapping of Ar on Pt surfaces (Head-Gordon et al., 1990).
- The results from the simulations have been implemented in feature scale modeling of film coverage in the metallization of micron-sized features (vias and trenches) in integrated circuits.